Inadequacy of Taylor series for perturbation expansion: a lesson from weak measurement

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Abstract

We all learnt from calculus textbooks that a Taylor expansion should be made consistently: all first-order terms should be grouped together, then all the second-order terms, etc. However, when applying perturbation theory to estimate probabilities, a common task in quantum mechanics, this automatic procedure can lead to nonpositive-definite probabilities. (Here, we are talking about probabilities that must be positive, as they can be inferred directly from the frequency of observed events, and not about intermediate functions, as Wigner quasiprobabilities, the inference of which from experimental data is a nontrivial task.) We demonstrate how to preserve the nonnegativity of probabilities at the cost of getting a bad grade in Calculus, and we show how the corrected expansion leads to a modification of the commonly accepted expressions for weak measurements, curing unphysical divergences at the same time. We provide the corrected formulas in the trivial case of an instantaneous interaction, the most commonly studied, and in the case of a finite-duration interaction during which the measured observable is not conserved. In the linear regime, the response of the detector is shown to be given by a generalized Kubo formula for a non-Hermitian perturbation.

WHAT IS A MEASUREMENT?

Some may have a very restricted idea of a measurement, limiting the concept to the case when a single observation on a system allows to infer total information about a dynamical quantity of interest in a second system that interacted with the first in a controlled way. For us, instead, a measurement is any act of inference about a system done by observing another system (which can be called indifferently the detector, the meter, the probe, the apparatus, or the ancilla) that has interacted with the measured system, even though this inference has some uncertainty connected to it.

From a strict philosophical view, we never observe anything but our sensations or perceptions, i.e. the consciousness of sensations, that are given to us in an immediate way, according to Kant,[1] who stated: "Things in space and time are given only in so far as they are perceptions (that is, representations accompanied by sensation)–therefore only through empirical representation". Thus, in principle, we should follow the observed system, and then the measuring apparatus that interacts with it, hence the visible electromagnetic fields that interact with the former, and then our retinas that interact with the e.m. field, etc., in a chain with a blurred end due to ill-defined terms such as "consciousness" and "sensation". As von Neumann noted,[2] in quantum mechanics there is no need to go up this chain. Sometimes, it is sufficient to apply the rules of quantum mechanics directly to the system. This turns out to be the case of a projective measurement. Most of the other times, it is necessary to go up just one step, by describing both the system and the detecting apparatus. Consistency requires that the former case is a limiting case of the latter. It is important to remark that in this second case we can not make definite inferences about the system, but we have to leave some room for uncertainties. These uncertainties may be classical, in the sense that we do not know the exact state of the detector, that the readout has always some noise, etc. But they can also be quantum, if the detector is prepared in a superposition. Observing the consequences of the quantum nature of the detector, however, is not immediate.

In a seminal work,[3] Aharonov, Albert, and Vaidman showed that by having a weak interaction between system and apparatus, the average output of the latter could be much larger than the maximum eigenvalue of the observed quantity (times the amplification factor). Soon, it was realized[4] that the quantum nature of the detector was at the basis of this phenomenon, as constructive interference in the probability tails for the readout led to the large

average values of the output. This does not always happen, however: the observed system must subsequently undergo a second measurement, on the output of which the result of the first one is conditioned. This procedure is known as postselection. When the postselected state is almost orthogonal to the initial state of the system, the anomalous average output is observed. However, as the initial state of the system is only slightly perturbed by the weak interaction, the probability of a successful postselection is very small in this regime, so that one has to be patient and collect a huge amount of data, before getting his reward.

The (rare) amplification of the output certainly contributed to popularize the subject of weak measurement, but whether it lead to a net gain in signal-to-noise or in the amplification is somewhat controversial.[5,6] The worth of postselected weak measurements, instead, could reside in its allowing sequential or joint non-projective measurements,[7–11] in its providing new techniques to perform quantum state tomography,[12–15] or in its possibly leading to the disembodiment of dynamical properties from their physical vehicles.[16–19]

METHODS

The weak measurement formalism[3] is but perturbation theory applied to the composite system formed by the measured system and by a second quantum system, the detector. To avoid confusion, we shall say "total system" when referring to both the detector and the measured system, and "system" when referring to this latter. The perturbation is done in the interaction between the two subsystems, while the evolution due to the free Hamiltonians is considered to be easily computable. Furthermore, contrary to textbook perturbation theory, the formalism is applied to conditional probabilities, after a postselection on the system is done. As observable probabilities are nonnegative-definite, particular care should be taken while making the perturbative expansion, in order to preserve this essential property. In particular, as we show below, the common knowledge that all terms of a given order are to be grouped together does not apply.

A simple case: instantaneous interaction.

For simplicity, we make the following hypotheses:

1. the interaction between system and detector is a (von Neumann) instantaneous inter-

action;

2. the probability is calculated immediately after the interaction;

3. the preparation of the system and the probe $\rho_i \otimes \rho_0$ is known immediately before the interaction;

4. the postselection in the state $\rho_f \otimes \mathbb{1}$ is made immediately after the interaction.

The extension to an arbitrary case is obvious, except perhaps for point 1.[20,21]

The joint probability of postselecting the total system in $\rho_f \otimes |R\rangle\langle R|$ (we assume that the measurement on the detector is sharp, so that Born's rule applies) is then

$$\mathcal{P}(R, \rho_f) = \mathrm{Tr}\left[(\rho_f \otimes |R\rangle\langle R|)\mathcal{U}(\rho_i \otimes \rho_0)\mathcal{U}^\dagger\right], \tag{1}$$

with the time-evolution $\mathcal{U} = \exp[i\lambda \hat{A}\hat{X}]$. We kept the interaction in the von Neumann protocol, with $\hat{A}$ observable of the system and $\hat{X}$ observable of the meter and λ a coupling constant. However, notice that, contrary to the von Neumann protocol, we are not assuming that the readout variable $\hat{R}$ is conjugated to $\hat{X}$, nor that the meter is initially in a sharp state of the readout $\rho_0 \simeq |R = 0\rangle\langle R = 0|$.

The probability of postselecting the system in ρ_f is

$$\mathcal{P}(\rho_f) = \sum_R \mathcal{P}(R, \rho_f). \tag{2}$$

Let us apply perturbation theory , to Eqs. (1) and (2), including up to first order terms in the propagator

$$\mathcal{P}(R, \rho_f) \simeq \mathrm{Tr}\left\{(\rho_f \otimes |R\rangle\langle R|)\left[1 + i\lambda\hat{A}\hat{X}\right](\rho_i \otimes \rho_0)\left[1 - i\lambda\hat{A}\hat{X}\right]\right\}, \tag{3}$$

$$\mathcal{P}(\rho_f) \simeq \mathrm{Tr}\left\{(\rho_f \otimes \mathbb{1})\left[1 + i\lambda\hat{A}\hat{X}\right](\rho_i \otimes \rho_0)\left[1 - i\lambda\hat{A}\hat{X}\right]\right\}. \tag{4}$$

The textbook calculus approach would be, e.g., to retain the first order terms,

$$\mathcal{P}_1(R, \rho_f) = \mathrm{Tr}_S[\rho_f\rho_i]\langle R|\rho_0|R\rangle + \left\{i\lambda\,\mathrm{Tr}_S[\rho_f\hat{A}\rho_i]\langle R|\hat{X}\rho_0|R\rangle + c.c.\right\}, \tag{5}$$

$$\mathcal{P}_1(\rho_f) = \mathrm{Tr}_S[\rho_f\rho_i] + \left\{i\lambda\,\mathrm{Tr}_S[\rho_f\hat{A}\rho_i]\,\mathrm{Tr}_D[\hat{X}\rho_0] + c.c.\right\}. \tag{6}$$

However, the above expressions do not preserve the positivity of the probability, since they are not of the form $\mathcal{P} = \mathrm{Tr}\,[EU_1FU_1^\dagger]$ with E, F positive operators and U_1 an arbitrary

operator. True, the neglected terms are $\mathcal{O}(\lambda^2)$, but nevertheless the probability could turn negative for some values of ρ_f and R if to lowest order $\mathcal{P} \ll 1$. This can occur if λ is somewhat largish. The correct way to make the expansion is to keep the product of the first order terms in $\mathcal{U}$ and $\mathcal{U}^\dagger$, giving

$$\mathcal{P}(R,\rho_f) \simeq \mathrm{Tr}_S[\rho_f\rho_i]\langle R|\rho_0|R\rangle + \lambda\left\{i\,\mathrm{Tr}_S[\rho_f\hat{A}\rho_i]\langle R|\hat{X}\rho_0|R\rangle + c.c.\right\} \\ + \lambda^2\,\mathrm{Tr}_S[\rho_f\hat{A}\rho_i\hat{A}]\langle R|\hat{X}\rho_0\hat{X}|R\rangle, \tag{7}$$

$$\mathcal{P}(\rho_f) \simeq \mathrm{Tr}_S[\rho_f\rho_i] + \left\{i\lambda\,\mathrm{Tr}_S[\rho_f\hat{A}\rho_i]\,\mathrm{Tr}_D[\hat{X}\rho_0] + c.c.\right\} + \lambda^2\,\mathrm{Tr}_S[\rho_f\hat{A}\rho_i\hat{A}]\,\mathrm{Tr}_D[\hat{X}^2\rho_0]. \tag{8}$$

Thus, up to "first order", the system enters the probabilities with three terms: the overlap $O = \mathrm{Tr}_S[\rho_f\rho_i]$, the complex number $A_w = \mathrm{Tr}_S[\rho_f\hat{A}\rho_i]/O$ and the real number $B_w = \mathrm{Tr}_S[\rho_f\hat{A}\rho_i\hat{A}]/O$. If one considers, as usually done in the context of weak measurement, the conditional probability $\mathcal{Q}(R) = \mathcal{P}(R,\rho_f)/\mathcal{P}(\rho_f)$ and its related averages, the overlap O can be simplified between numerator and denominator. While mathematician will shudder in disgust, O may as well be 0, and the formulas still be valid, in the sense that in this limit B_w is overwhelmingly large compared to A_w, in both the numerator and the denominator. Another point in favor of this improved expansion is that while OA_w tends to 0 for $O \to 0$, the product OB_w stays finite, excluding some trivial cases for which the probability of post-selection is exactly null. For this reason, the expansion is robust for any preparation and postselection of the system.

But what does a naïve application of Taylor series, as learnt from Calculus, prescribes? Since we are including a second order term, according to the prescription, for consistency we should expand the propagator up to second-order, and retain terms like $\lambda^2\,\mathrm{Tr}\,(\rho_f \otimes |R\rangle\langle R|)\hat{A}^2\hat{X}^2(\rho_i\otimes\rho_0)$. We did this in a previous paper,[22] where we stated erroneously that the reason to neglect these terms, which give rise to a complex number $C_w = \mathrm{Tr}_S[\rho_f\hat{A}^2\rho_i]/O$, was that the second order correction becomes relevant only in the regime $C_w \ll B_w$. From the discussion above, instead, it can be seen that dropping of C_w is justified by the positive-definiteness of the probability. If we wanted to retain terms $\lambda^2\hat{A}^2\hat{X}^2$ in the propagator $\mathcal{U}$, we should retain some λ^3 and λ^4 terms in the probability. Paradoxically, as shown in Fig. 1, including the second order terms in the Taylor series according to the textbook prescription may make the probability more negative than the first order approximation.

Finally, the conditional average of an arbitrary observable $\hat{R}$ is obtained by integration,

$$\langle R\rangle \simeq \frac{\langle \hat{R}\rangle_0 + i\lambda A'_w \langle[\hat{R},\hat{X}]\rangle_0 - \lambda A''_w\langle\{\hat{R},\hat{X}\}\rangle_0 + \lambda^2 B_w \langle \hat{X}\hat{R}\hat{X}\rangle_0}{1-2\lambda A''_w\langle\hat{X}\rangle_0 + \lambda^2 B_w\langle\hat{X}^2\rangle_0}, \tag{9}$$

where $\langle\hat{M}\rangle_0 = \mathrm{Tr}_D[\hat{M}\hat{\rho}_0]$, $[\hat{M},\hat{N}] = \hat{M}\hat{N} - \hat{N}\hat{M}$, and $\{\hat{M},\hat{N}\} = \hat{M}\hat{N} + \hat{N}\hat{M}$, $A'_w = \mathrm{Re}(A_w)$ and $A''_w = \mathrm{Im}(A_w)$. Notice that we did not assume anything about the spectrum of $\hat{R}$: it may be continuous, discrete, or mixed.

In particular, in the limit $\lambda A''_w\langle\hat{X}\rangle_0 \ll 1$, $\lambda^2 B_w\langle\hat{X}^2\rangle_0 \ll 1$, it may be possible to retain the first order terms, provided that B_w is not too large, i.e., provided the overlap between the preparation and the postselection is not too small. Then the result of Ref. 23 is recovered

$$\langle R\rangle \simeq \langle\hat{R}\rangle_0 + i\lambda A'_w\langle[\hat{R},\hat{X}]\rangle_0 - \lambda A''_w\left[\langle\{\hat{R},\hat{X}\}\rangle_0 - 2\langle\hat{R}\rangle_0\langle\hat{X}\rangle_0\right]. \tag{10}$$

Remark the appearance of the symmetrized correlator. In any case, there is no a priori reason to prefer a polynomial in λ to the rational function of Eq. (9). In particular, it may seem that making a first order approximation, while inadequate for a probability, that is nonnegative, could be appropriate for the average value. However, let us consider the following extreme example: the detector is a two-level system, whose output can be $R = -1$ or $R = +1$. The average value is a simple function of the probability $\langle R\rangle = 2P(R=1) - 1$. If the probability takes a negative value, $\langle R\rangle$ becomes smaller than -1, which is impossible.

General case: Interaction with a finite duration.

Now we lift the hypothesis 1 made in the previous subsection, i.e. we allow the interaction to last a finite time. Contrary to previous works,[20,21] we shall not assume that $\hat{A}$ or $\hat{R}$ is conserved. This generalization is particularly interested in prospective solid state realizations of weak measurement.[24–30] The interaction is shaped by a function $g(t)$, satisfying $\int dt g(t) = 1$ and vanishing outside a time window $[0,\tau]$. For convenience, we factor out the interaction strength λ, so that

$$H_{int} = -\hbar\lambda g(t)\hat{A}\hat{X}. \tag{11}$$

Hence, the time-evolution operator is

$$\mathcal{U} = \mathcal{U}_0\,\mathcal{T}\left\{\exp\left[i\lambda\int_0^\tau dt\, g(t)\hat{A}(t)\hat{X}(t)\right]\right\}, \tag{12}$$

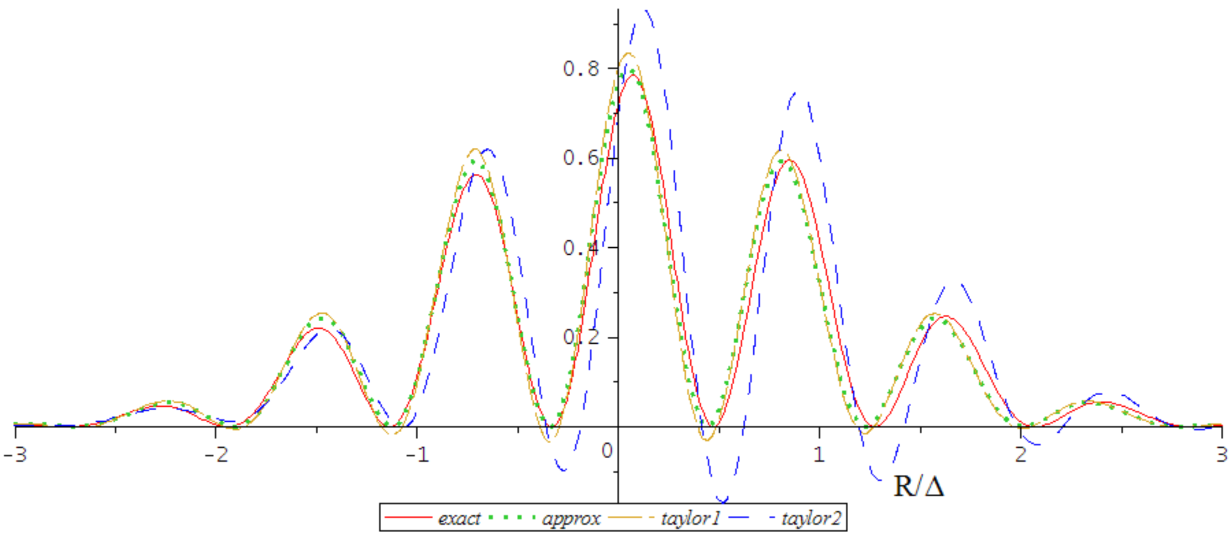

FIG. 1. **Comparison between Taylor series and the controlled approximation.** The plot shows the probability for a measurement of the z-component of a spin 1/2. The solid line represents the exact result, the dotted line the controlled approximation given by the ratio of Eq. (7) and Eq. (8), the dot-dashed line the first-order Taylor series, and the long-dashed line the second-order Taylor series. The spin is prepared in a pure state making an angle $\pi/3$ with the z-axis, measured weakly, then postselected in a state making an angle $\pi/2$ with the z-axis and coplanar with z and the preparation polarization. The probe was initially prepared in the pure state $\psi(R) = \cos(4R/\Delta)\exp[-R^2/4\Delta^2]$. The interaction between the probe and the spin was $H_{int} = -\hbar\delta(t)\lambda\hat{\sigma}_z\hat{X}$, with $[\hat{X}, \hat{R}] = i$. We took $\lambda = 0.2\Delta$.

with $\mathcal{T}$ time-ordering, $\mathcal{U}_\tau^{(0)} = \mathcal{U}_\tau^{(S)} \otimes \mathcal{U}_\tau^{(D)}$ free evolution of system and detector, while $\hat{A}(t) = \mathcal{U}_t^{(S)\dagger}\hat{A}\mathcal{U}_t^{(S)}$ $\hat{X}(t) = \mathcal{U}_t^{(D)\dagger}\hat{X}\mathcal{U}_t^{(D)}$ are the operators in the interaction representation. As in the previous subsection, we make a controlled expansion to "first order" of the joint probability:

$$
\begin{aligned}
\mathcal{P}(R, \rho_f) \simeq \mathrm{Tr}\Big\{&\mathcal{U}_\tau^{(0)\dagger}\left(\rho_f \otimes |R\rangle\langle R|\right)\mathcal{U}_\tau^{(0)}\left[1 + i\lambda\int_0^\tau dt\, g(t)\hat{A}(t)\hat{X}(t)\right] \\
&\times\left(\rho_i \otimes \rho_0\right)\left[1 - i\lambda\int_0^\tau dt\, g(t)\hat{A}(t)\hat{X}(t)\right]\Big\}, \\
\simeq \mathrm{Tr}_S[\rho_f(\tau)\rho_i]\Big\{&\langle R(\tau)|\rho_0|R(\tau)\rangle + \lambda\left[i\int_0^\tau dt\, g(t)A_w(t)\langle R(\tau)|\hat{X}(t)\rho_0|R(\tau)\rangle + c.c\right] \\
&+ \lambda^2\iint_0^\tau dtdt' g(t)g(t')B_w(t,t')\langle R(\tau)|\hat{X}(t)\rho_0\hat{X}(t')|R(\tau)\rangle\Big\}. \qquad (13)
\end{aligned}
$$

We put $|R(\tau)\rangle\langle R(\tau)| = \mathcal{U}_\tau^{(D)\dagger}|R\rangle\langle R|\mathcal{U}_\tau^{(D)}$ and $\rho_f(\tau) = \mathcal{U}_\tau^{(S)\dagger}\rho_f\mathcal{U}_\tau^{(S)}$ the state $|R\rangle\langle R|$ and ρ_f, respectively, propagated backwards in time to the beginning of the interaction, and defined the time-dependent weak values

$$A_w(t) = \frac{\mathrm{Tr}_S[\rho_f(\tau)\hat{A}(t)\rho_i]}{\mathrm{Tr}_S[\rho_f(\tau)\rho_i]}, \tag{14}$$

$$B_w(t,t') = \frac{\mathrm{Tr}_S[\rho_f(\tau)\hat{A}(t)\rho_i\hat{A}(t')]}{\mathrm{Tr}_S[\rho_f(\tau)\rho_i]}. \tag{15}$$

Consequently, the probability of postselection is

$$\begin{aligned}\mathcal{P}(\rho_f) \simeq \mathrm{Tr}_S[\rho_f(\tau)\rho_i]\bigg\{1 - 2\lambda\int_0^\tau dt\, g(t)\langle\hat{X}(t)\rangle_0 A_w''(t) \\ + \lambda^2\int_0^\tau\int_0^\tau dtdt' g(t)g(t')\langle\hat{X}(t')\hat{X}(t)\rangle_0 B_w(t,t')\bigg\}.\end{aligned} \tag{16}$$

The conditional average is then

$$\begin{aligned}\langle R\rangle \simeq \bigg\{1 - 2\lambda\int_0^\tau dt\, g(t)\langle\hat{X}(t)\rangle_0 A_w''(t) + \lambda^2\iint_0^\tau dtdt' g(t)g(t')\langle\hat{X}(t')\hat{X}(t)\rangle_0 B_w(t,t')\bigg\}^{-1} \\ \times\bigg\{\langle\hat{R}(\tau)\rangle_0 + \lambda\int_0^\tau dt\, g(t)\left(A_w'(t)\langle i[\hat{R}(\tau),\hat{X}(t)]\rangle_0 - A_w''(t)\langle\{\hat{R}(\tau),\hat{X}(t)\}\rangle_0\right) \\ + \lambda^2\iint_0^\tau dtdt' g(t)g(t')B_w(t,t')\langle\hat{X}(t')\hat{R}(\tau)\hat{X}(t)\rangle_0\bigg\}.\end{aligned} \tag{17}$$

In the linear regime, we have the modified Kubo formula

$$\langle R\rangle \simeq \langle\hat{R}(\tau)\rangle_0 + i\int_0^\tau dt\,\langle\hat{W}(t)\hat{R}(\tau) - \hat{R}(\tau)\hat{W}^\dagger(t)\rangle_0 \tag{18}$$

with the non-Hermitian operator

$$\hat{W}(t) = \lambda g(t)A_w(t)[\hat{X}(t) - \langle\hat{X}(t)\rangle_0]. \tag{19}$$

Notice that when no postselection is made, $\rho_f = \mathbb{1}$, the weak value $A_w(t) = \langle\hat{A}(t)\rangle_i$ is real, and the ordinary Kubo formula is recovered.

CONCLUSIONS.

We have derived a general formula for the weak measurement, providing positive-definite probabilities by construction, and giving an interpolation to the average output of an arbitrary variable for arbitrary preparation and postselection.

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